ACS Sustainable Chemistry and Engineering, 2017, vol.5, N1, pages 911-921

1,2,3-Trimethoxypropane: A Glycerol-Derived Physical Solvent for CO2 Absorption

Flowers B., Mittenthal M., Jenkins A., Wallace D., Whitley J., Dennis G., Wang M., Turner C., Emel'Yanenko V., Verevkin S., Bara J.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2016 American Chemical Society. 1,2,3-Trimethoxypropane (1,2,3-TMP) is the trimethyl ether of propane-1,2,3-triol, better known as glycerol, which can be derived from triglycerides originating from either plant or animal sources. Despite its simple structure and the ubiquity of its glycerol precursor, successful synthesis of 1,2,3-TMP was only recently reported in the literature, with studies suggesting it may be a "green" and nontoxic alternative to solvents such as diglyme, a constitutional isomer. However, no thermophysical properties of 1,2,3-TMP have yet been reported. Furthermore, the structure of 1,2,3-TMP is also analogous to polyether solvents used in the Selexol process for removal of CO 2 and other "acid" gases from CH 4 , H 2 , etc. As such, examining the solubility of CO 2 in 1,2,3-TMP is also of interest. This work details our initial studies and characterization of 1,2,3-TMP as a physical solvent for CO 2 absorption, as well as the characterization of its density, viscosity, and vapor pressure with respect to temperature. 1,2,3-TMP exhibits favorable properties, and glycerol-derived triethers warrant deeper consideration as new solvents for CO 2 absorption and other gas treating applications.

http://dx.doi.org/10.1021/acssuschemeng.6b02231

Keywords

Glycerol, Green chemistry, Physical solvent, Precombustion CO capture 2, Selexol

References

[1] Rochelle, G. T. Amine Scrubbing for CO Capture Science 2009, 325 (5948) 1652-1654 10.1126/science.1176731
[2] Burr, B.; Lyddon, L. A Comparison of Physical Solvents for Acid Gas Removal. In Gas Processors' Association Convention; Grapevine, TX, 2008.
[3] Bucklin, R. W.; Schendel, R. L. Physical Solvent Processes Can Be Very Useful for Acid Gas Removal Applications Energy Progress 1984, 4 (3) 137-142
[4] Astarita, G.; Savage, D. W.; Bisio, A. Gas Treating with Chemical Solvents; John Wiley & Sons: New York, 1983.
[5] Kidnay, A. J.; Parrish, W. R. Fundamentals of Natural Gas Processing; CRC Press: Taylor & Francis Group: Boca Raton, FL, 2006.
[6] Tennyson, R. N.; Schaaf, R. P. Guidelines can help choose proper process for gas-treating plants Oil Gas J. 1977, 75 (2) 78-86
[7] Miller, B. G. 7-Clean Coal Technologies for Advanced Power Generation. In Clean Coal Engineering Technology; Butterworth-Heinemann: Boston, 2011; pp 251-300.
[8] Lin, H. Q.; Freeman, B. D. Materials selection guidelines for membranes that remove CO2 from gas mixtures J. Mol. Struct. 2005, 739 (1-3) 57-74 10.1016/j.molstruc.2004.07.045

[9] NETL. DOE/NETL Advanced Carbon Dioxide Capture R&D Program: May 2013 Update. https://www.netl.doe.gov/File%20Library/Research/Coal/carbon%20capture/handbook/CO2-Capture-Tech-Update-2013.pdf (15 September 2016).

[10] Murrieta-Guevara, F.; Romero-Martinez, A.; Trejo, A. Solubilities of carbon dioxide and hydrogen sulfide in propylene carbonate, N-methylpyrrolidone and sulfolane Fluid Phase Equilib. 1988, 44 (1) 105-115 10.1016/0378-3812(88)80106-7

[11] Shannon, M. S.; Tedstone, J. M.; Danielsen, S. P. O.; Bara, J. E. Evaluation of Alkylimidazoles as Physical Solvents for CO/CH Separation Ind. Eng. Chem. Res. 2012, 51 (1) 515-522 10.1021/ie202111k

[12] Shannon, M. S.; Tedstone, J. M.; Danielsen, S. P. O.; Hindman, M. S.; Irvin, A. C.; Bara, J. E. Free Volume as the Basis of Gas Solubility and Selectivity in Imidazolium-Based Ionic Liquids Ind. Eng. Chem. Res. 2012, 51 (15) 5565-5576 10.1021/ie202916e

[13] Shannon, M. S.; Bara, J. E. Properties of Alkylimidazoles as Solvents for CO Capture and Comparisons to Imidazolium-Based Ionic Liquids Ind. Eng. Chem. Res. 2011, 50 (14) 8665-8677 10.1021/ie200259h

[14] Bara, J. E.; Camper, D. E.; Gin, D. L.; Noble, R. D. Room-Temperature Ionic Liquids and Composite Materials: Platform Technologies for CO Capture Acc. Chem. Res. 2010, 43 (1) 152-159 10.1021/ar9001747

[15] Bara, J. E.; Carlisle, T. K.; Gabriel, C. J.; Camper, D.; Finotello, A.; Gin, D. L.; Noble, R. D. Guide to CO Separations in Imidazolium-Based Room-Temperature Ionic Liquids Ind. Eng. Chem. Res. 2009, 48 (6) 2739-2751 10.1021/ie8016237

[16] Carvalho, P. J.; Kurnia, K. A.; Coutinho, J. A. P. Dispelling some myths about the CO solubility in ionic liquids Phys. Chem. Chem. Phys. 2016, 18 (22) 14757-14771 10.1039/C6CP01896C

[17] Carvalho, P. J.; Coutinho, J. A. P. On the Nonideality of CO Solutions in Ionic Liquids and Other Low Volatile Solvents J. Phys. Chem. Lett. 2010, 1 (4) 774-780 10.1021/jz100009c

[18] Bara, J. E.; Gabriel, C. J.; Carlisle, T. K.; Camper, D. E.; Finotello, A.; Gin, D. L.; Noble, R. D. Gas separations in fluoroalkyl-functionalized room-temperature ionic liquids using supported liquid membranes Chem. Eng. J. 2009, 147 (1) 43-50 10.1016/j.cej.2008.11.021

[19] Carlisle, T. K.; Bara, J. E.; Gabriel, C. J.; Noble, R. D.; Gin, D. L. Interpretation of CO solubility and selectivity in nitrile-functionalized room-temperature ionic liquids using a group contribution approach Ind. Eng. Chem. Res. 2008, 47 (18) 7005-7012 10.1021/ie8001217

[20] Bara, J. E.; Gabriel, C. J.; Lessmann, S.; Carlisle, T. K.; Finotello, A.; Gin, D. L.; Noble, R. D. Enhanced CO separation selectivity in oligo(ethylene glycol) functionalized room-temperature ionic liquids Ind. Eng. Chem. Res. 2007, 46 (16) 5380-5386 10.1021/ie070437g

[21] Shannon, M. S.; Tedstone, J. M.; Danielsen, S. P. O.; Hindman, M. S.; Bara, J. E. Properties and Performance of Ether-Functionalized Imidazoles as Physical Solvents for CO Separations Energy Fuels 2013, 27 (6) 3349-3357 10.1021/ef400362b

[22] Anthony, J. L.; Anderson, J. L.; Maginn, E. J.; Brennecke, J. F. Anion effects on gas solubility in ionic liquids J. Phys. Chem. B 2005, 109 (13) 6366-6374 10.1021/jp046404l

[23] Shiflett, M. B.; Elliott, B. A.; Lustig, S. R.; Sabesan, S.; Kelkar, M. S.; Yokozeki, A. Phase Behavior of CO in Room-Temperature Ionic Liquid 1-Ethyl-3-Ethylimidazolium Acetate ChemPhysChem 2012, 13 (7) 1806-1817 10.1002/cphc.201200023

[24] Shiflett, M. B.; Niehaus, A. M. S.; Yokozeki, A. Separation of CO and HS Using Room-Temperature Ionic Liquid [bmim][MeSO] J. Chem. Eng. Data 2010, 55 (11) 4785-4793 10.1021/je1004005

[25] Shiflett, M. B.; Yokozeki, A. Phase Behavior of Carbon Dioxide in Ionic Liquids: [emim][Acetate], [emim][Trifluoroacetate], and [emim][Acetate] + [emim][Trifluoroacetate] Mixtures J. Chem. Eng. Data 2009, 54 (1) 108-114 10.1021/je800701j

[26] Yokozeki, A.; Shiflett, M. B.; Junk, C. P.; Grieco, L. M.; Foo, T. Physical and Chemical Absorptions of Carbon Dioxide in Room-Temperature Ionic Liquids J. Phys. Chem. B 2008, 112 (51) 16654-16663 10.1021/jp805784u

[27] Cui, Z.; de Montigny, D. Part 7: A review of CO capture using hollow fiber membrane contactors Carbon Manage. 2013, 4 (1) 69-89 10.4155/cmt.12.73

[28] Li, S.; Rocha, D. J.; Zhou, S. J.; Meyer, H. S.; Bikson, B.; Ding, Y. Post-combustion CO capture using super-hydrophobic, polyether ether ketone, hollow fiber membrane contactors J. Membr. Sci. 2013, 430, 79-86 10.1016/j.memsci.2012.12.001

[29] Favre, E.; Svendsen, H. F. Membrane contactors for intensified post-combustion carbon dioxide capture by gas-liquid absorption processes J. Membr. Sci. 2012, 407-408, 1-7 10.1016/j.memsci.2012.03.019

[30] Zhou, S. J.; Li, S.; Meyer, H.; Bikson, B.; Ding, Y. Hybrid membrane absorption process for post combustion, CO capture Int. Tech. Conf. Clean Coal Fuel Syst. 2012, 37, 129-139

[31] Li, J.-L.; Chen, B.-H. Review of CO absorption using chemical solvents in hollow fiber membrane contactors Sep. Purif. Technol. 2005, 41 (2) 109-122 10.1016/j.seppur.2004.09.008

[32] Gabelman, A.; Hwang, S.-T. Hollow fiber membrane contactors J. Membr. Sci. 1999, 159 (1-2) 61-106 10.1016/S0376-7388(99)00040-X

[33] Rangwala, H. A. Absorption of carbon dioxide into aqueous solutions using hollow fiber membrane contactors J. Membr. Sci. 1996, 112 (2) 229-40 10.1016/0376-7388(95)00293-6

[34] Wijmans, J. G.; Baker, R. W. The solution-diffusion model: a review J. Membr. Sci. 1995, 107 (1-2) 1-21 10.1016/0376-7388(95)00102-I

[35] de Queiroz F. Araújo, O.; de Medeiros, J. L.; Alves, R. M. B. CO Utilization: A Process Systems Engineering Vision. In CO Sequestration and Valorization; Estevez, V., Ed.; Intech, 2014.

[36] Appleby, D. B. In Glycerol; AOCS Press, 2005; pp 264-276.

[37] Sheely, M. L. Glycerol Viscosity Tables Ind. Eng. Chem. 1932, 24 (9) 1060-1064 10.1021/ie50273a022

[38] Sutter, M.; Dayoub, W.; Métay, E.; Raoul, Y.; Lemaire, M. 1,2,3-Trimethoxypropane and Glycerol Ethers as Bio-Sourced Solvents from Glycerol. Synthesis by Solvent-Free Phase-Transfer Catalysis and Utilization as an Alternative Solvent in Chemical Transformations ChemCatChem 2013, 5 (10) 2893-2904 10.1002/cctc.201300458

[39] Sutter, M.; Pehlivan, L.; Lafon, R.; Dayoub, W.; Raoul, Y.; Metay, E.; Lemaire, M. 1,2,3-Trimethoxypropane, a glycerol-based solvent with low toxicity: new utilization for the reduction of nitrile, nitro, ester, and acid functional groups with TMDS and a metal catalyst Green Chem. 2013, 15 (11) 3020-3026 10.1039/c3gc41082j

[40] Henni, A.; Tontiwachwuthikul, P.; Chakma, A. Solubilities of carbon dioxide in polyethylene glycol ethers Can. J. Chem. Eng. 2005, 83 (2) 358-361 10.1002/cjce.5450830224

[41] Sutter, M.; Silva, E. D.; Duguet, N.; Raoul, Y.; Métay, E.; Lemaire, M. Glycerol Ether Synthesis: A Bench Test for Green Chemistry Concepts and Technologies Chem. Rev. 2015, 115 (16) 8609-8651 10.1021/cr5004002

[42] Alder, C. M.; Hayler, J. D.; Henderson, R. K.; Redman, A. M.; Shukla, L.; Shuster, L. E.; Sneddon, H. F. Updating and further expanding GSK's solvent sustainability guide Green Chem. 2016, 18 (13) 3879-3890 10.1039/C6GC00611F

[43] Trost, B. M. The Atom Economy-A Search for Synthetic Efficiency Science 1991, 254 (5037) 1471-1477 10.1126/science.1962206

[44] Garist, I. V.; Verevkin, S. P.; Samarov, A. A.; Bara, J. E.; Hindman, M. S.; Danielsen, S. P. O. Building Blocks for Ionic Liquids: Vapor Pressures and Vaporization Enthalpies of Alkoxy Derivatives of Imidazole and Benzimidazole Ind. Eng. Chem. Res. 2012, 51 (47) 15517-15524 10.1021/ie302383t

[45] Emel'yanenko, V. N.; Portnova, S. V.; Verevkin, S. P.; Skrzypczak, A.; Schubert, T. Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles J. Chem. Thermodyn. 2011, 43 (10) 1500-1505 10.1016/j.jct.2011.05.004

[46] Verevkin, S. P.; Zaitsau, D. H.; Emel'yanenko, V. N.; Paulechka, Y. U.; Blokhin, A. V.; Bazyleva, A. B.; Kabo, G. J. Thermodynamics of Ionic Liquids Precursors: 1-Methylimidazole J. Phys. Chem. B 2011, 115 (15) 4404-4411 10.1021/jp201752j

[47] Verevkin, S. P.; Emel'yanenko, V. N. Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters Fluid Phase Equilib. 2008, 266 (1-2) 64-75 10.1016/j.fluid.2008.02.001

[48] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian09, Revision A.1; Wallingford, CT, 2009.

[49] Becke, A. D. Density-Functional Thermochemistry 0.3. The Role of Exact Exchange J. Chem. Phys. 1993, 98 (7) 5648-5652 10.1063/1.464913

[50] Lee, C. T.; Yang, W. T.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron-Density Phys. Rev. B: Condens. Matter Mater. Phys. 1988, 37 (2) 785-789 10.1103/PhysRevB.37.785

[51] Breneman, C. M.; Wiberg, K. B. Determining atom-centered monopoles from molecular electrostatic potentials. The need for high sampling density in formamide conformational analysis J. Comput. Chem. 1990, 11 (3) 361-373 10.1002/jcc.540110311

[52] Bara, J. E.; Moon, J. D.; Reclusado, K. R.; Whitley, J. W. COSMOTherm as a Tool for Estimating the Thermophysical Properties of Alkylimidazoles as Solvents for CO Separations Ind. Eng. Chem. Res. 2013, 52 (15) 5498-5506 10.1021/ie400094h

[53] Horne, W. J.; Shannon, M. S.; Bara, J. E. Correlating fractional free volume to CO selectivity in [Rmim][TfN] ionic liquids J. Chem. Thermodyn. 2014, 77, 190-196 10.1016/j.jct.2014.03.012

[54] Shannon, M. S.; Irvin, A. C.; Liu, H.; Moon, J. D.; Hindman, M. S.; Turner, C. H.; Bara, J. E. Chemical and Physical Absorption of SO by N-Functionalized Imidazoles: Experimental Results and Molecular-level Insight Ind. Eng. Chem. Res. 2015, 54 (1) 462-471 10.1021/ie503752h

[55] Ahlrichs, R.; Bär, M.; Häser, M.; Horn, H.; Kölmel, C. Electronic structure calculations on workstation computers: The program system turbomole Chem. Phys. Lett. 1989, 162 (3) 165-169 10.1016/0009-2614(89)85118-8

[56] Schafer, A.; Huber, C.; Ahlrichs, R. Fully optimized contracted Gaussian basis sets of triple zeta valence quality for atoms Li to Kr J. Chem. Phys. 1994, 100 (8) 5829-5835 10.1063/1.467146

[57] Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior Phys. Rev. A: At., Mol., Opt. Phys. 1988, 38 (6) 3098-3100 10.1103/PhysRevA.38.3098

[58] Perdew, J. P. Density-functional approximation for the correlation energy of the inhomogeneous electron gas Phys. Rev. B: Condens. Matter Mater. Phys. 1986, 33 (12) 8822-8824 10.1103/PhysRevB.33.8822

[59] Valtz, A.; Coquelet, C.; Boukais-Belaribi, G.; Dahmani, A.; Belaribi, F. B. Volumetric Properties of Binary Mixtures of 1,2-Dichloroethane with Polyethers from (283.15 to 333.15) K and at Atmospheric Pressure J. Chem. Eng. Data 2011, 56 (4) 1629-1657 10.1021/je101361u

[60] Finotello, A.; Bara, J. E.; Camper, D.; Noble, R. D. Room-temperature ionic liquids: Temperature dependence of gas solubility selectivity Ind. Eng. Chem. Res. 2008, 47 (10) 3453-3459 10.1021/ie0704142

[61] Stull, D. R. Vapor Pressure of Pure Substances. Organic and Inorganic Compounds Ind. Eng. Chem. 1947, 39 (4) 517-540 10.1021/ie50448a022

[62] Li, D.; Fang, W.; Xie, W.; Xing, Y.; Guo, Y.; Lin, R. Measurements on Vapor Pressure and Thermal Conductivity for Pseudo-binary Systems of a Hydrocarbon Fuel with Ethylene and Diethylene Glycol Dimethyl Ethers Energy Fuels 2009, 23 (2) 794-798 10.1021/ef8007163

[63] Clarke, E. C. W.; Glew, D. N. Evaluation of thermodynamic functions from equilibrium constants Trans. Faraday Soc. 1966, 62 (0) 539-547 10.1039/tf9666200539

[64] Nichols, G.; Orf, J.; Reiter, S. M.; Chickos, J.; Gokel, G. W. The vaporization enthalpies of some crown and polyethers by correlation gas chromatography Thermochim. Acta 2000, 346 (1-2) 15-28 10.1016/S0040-6031(99)00405-0

[65] Jalili, A. H.; Shokouhi, M.; Samani, F.; Hosseini-Jenab, M. Measuring the solubility of CO and HS in sulfolane and the density and viscosity of saturated liquid binary mixtures of (sulfolane + CO2) and (sulfolane + HS) J. Chem. Thermodyn. 2015, 85, 13-25 10.1016/j.jct.2015.01.001

[66] Lebeuf, R.; Illous, E.; Dussenne, C.; Molinier, V.; Silva, E. D.; Lemaire, M.; Aubry, J.-M. Solvo-Surfactant Properties of Dialkyl Glycerol Ethers: Application as Eco-Friendly Extractants of Plant Material through a Novel Hydrotropic Cloud Point Extraction (HCPE) Process ACS Sustainable Chem. Eng. 2016, 4 (9) 4815-4823 10.1021/acssuschemeng.6b01101

[67] Mandai, T.; Yoshida, K.; Tsuzuki, S.; Nozawa, R.; Masu, H.; Ueno, K.; Dokko, K.; Watanabe, M. Effect of Ionic Size on Solvate Stability of Glyme-Based Solvate Ionic Liquids J. Phys. Chem. B 2015, 119 (4) 1523-1534 10.1021/jp508100s

[68] Terada, S.; Mandai, T.; Nozawa, R.; Yoshida, K.; Ueno, K.; Tsuzuki, S.; Dokko, K.; Watanabe, M. Physicochemical properties of pentaglyme-sodium bis(trifluoromethanesulfonyl)amide solvate ionic liquid Phys. Chem. Chem. Phys. 2014, 16 (23) 11737-11746 10.1039/c4cp00746h

[69] Zhang, C.; Ueno, K.; Yamazaki, A.; Yoshida, K.; Moon, H.; Mandai, T.; Umebayashi, Y.; Dokko, K.; Watanabe, M. Chelate Effects in Glyme/Lithium Bis(trifluoromethanesulfonyl)amide Solvate Ionic Liquids. I. Stability of Solvate Cations and Correlation with Electrolyte Properties J. Phys. Chem. B 2014, 118 (19) 5144-5153 10.1021/jp501319e

[70] Zhang, C.; Yamazaki, A.; Murai, J.; Park, J.-W.; Mandai, T.; Ueno, K.; Dokko, K.; Watanabe, M. Chelate Effects in Glyme/Lithium Bis(trifluoromethanesulfonyl)amide Solvate Ionic Liquids, Part 2: Importance of Solvate-Structure Stability for Electrolytes of Lithium Batteries J. Phys. Chem. C 2014, 118 (31) 17362-17373 10.1021/jp504099q